4-Cyclohexylphenylacetic acid 35889-00-0 | DTXSID60189446

Model Performance

	n .
Model	I)ata
Widdei	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 4.02e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.34e-01

Confidence level: 6.37e-01

Nearest Neighbors from the Training Set

Image not found

11-Bromoundecanoic acid

Measured: 2.00e-04 Predicted: 2.33e-04

Image not found

6-Phenylhexanoic acid

Measured: 2.50e-03 Predicted: 3.30e-03

Image not found

5-Phenylvaleric acid Measured: 3.42e-03 Predicted: 1.32e-02